CURRICULUM VITAE

KEITH M. BEARDMORE BSc (Hons), MSc, PhD

Personal Details:

Home Address:		Work Address: CMG, Motorola SPS, MS-B285
	711 West Manhattan Ave. #B	Los Alamos National Laboratory
	Santa Fe, New Mexico, 87501. USA.	Los Alamos, New Mexico, 87545. USA.
Telephone:	(505) 989-1343	(505) 667-0883
Fax:		(505) 665-1999
E-mail:	kbeardmore@cybermesa.net	Keith.Beardmore@Motorola.com
WWW:	http://www.cybermesa.com/∼kbeardmore/	http://cnls.lanl.gov/∼beardm/

Date of Birth:	13 August 1969
Place of Birth:	Bridgnorth, United Kingdom
Nationality:	British
U.S. Visa Status:	H-1B1 (Specialty Occupation)
Marital Status:	Single

Education:

- Department of Mathematical Sciences, Loughborough University of Technology,
  October 1992 - December 1995: **Ph.D.**,
  Ph.D. Thesis: "*Dynamical Simulation of Multicomponent Carbon Based Materials*".
- Department of Mathematical Sciences, Loughborough University of Technology,
  October 1991 - September 1992: **M.Sc. (distinction)**, title: *Industrial Mathematical Modelling*.
  Dissertation: "*Vibration Reduction for Helicopter Airframes by Structural Optimisation*".
- Department of Mathematical Sciences, University of Manchester Institute of Science and Technology,
  October 1987 - July 1990: **B.Sc. (2:1)**, title: *Pure and Applied Mathematics*.
- Bridgnorth Endowed School, Bridgnorth, Shropshire,
  September 1980 - July 1987: **6 A Levels**, including:
  Mathematics (A), Further Mathematics (A), Physics (A), Chemistry (B).

Awards:

1999: R&D 100 award for the **REED** project (http://bifrost.lanl.gov/∼reed/). REED-MD (for *Rare Event Enhanced Domain following Molecular Dynamics*), a predictive software tool for use in semiconductor design, was developed in association with Motorola and the Semiconductor Research Corporation.

This annual award program, run by the Illinois-based R&D Magazine, honors significant commercial promise in products, materials or processes developed by the international research and development community. Technologies are nominated in open competition and judged by technical experts to select the 100 most significant, unique or promising entries.

1997: Team Award (with Niels Grønbech Jensen) for **Excellence in Technology Transfer**.
Awarded for the **REED** project by the Civilian and Industrial Technologies Program Office, Los Alamos National Laboratory.

Professional Experience:

3/1999-present: Research Scientist, Semiconductor Products Sector, **Motorola**.
My research is currently concerned with atomic scale materials simulation.

1/1996-2/1999: Postdoctoral Fellow, Theoretical Division, **Los Alamos National Laboratory**.

Current Research Interests:

My principal interests are in the area of computational materials modeling, with emphasis on investigation of 'real world' problems, i.e., problems of experimental or industrial interest. Modeling is conducted on the atomic scale, using variants of the methods of classical and ab-initio molecular dynamics (MD) simulation. Such simulations are complex and computationally expensive. My research is divided between the development of empirical models of atomic interactions, and the realization of these models as computer programs. Much of this research is devoted to developing and coding efficient algorithms to reduce computational overhead, whilst maintaining a realistic system description.

My current research is focused on modeling radiation effects in materials
This is directly related to materials problems of importance to the semiconductor industry. Topics include; modeling of dopant implants in silicon, energetics of defects, behavior of polymer resists subject to ion implant, the interaction of clusters with surfaces, radiation damage thresholds, and irradiation induced stress creation and relaxation in thin films.

Experience & Skills:

I have a good knowledge of UNIX, Linux, Windows NT, Fortran and C, on both serial and parallel architectures, and have considerable experience in the use of computer visualization and animation. I am currently system administrator for NT/Linux computers and Linux-Beowulf compute clusters. I was responsible for the design and construction of a significant part of WWW sites for the Department of Mathematical Sciences at Loughborough University, the Center for Nonlinear Studies at Los Alamos, and for my current research group at Motorola.

I have presented the results of my research work in oral and poster sessions at several international conferences. While at Loughborough University, I taught tutorial classes in mathematics for 1st and 2nd year undergraduate students. I was a principal organizer of the Workshop on Self-Assembling and Biomimetic Materials, held at Los Alamos in December 1997.

I am the author of two MD codes that are used by several research groups: MolDyn is a general purpose MD code for simulating ion and cluster impacts with crystal surfaces, that is now used at several universities, at Los Alamos, and within Motorola. REED is a specialized program for modeling ion implant into semiconductors, that is used by both industry and academia. I am also the principal maintainer of the REED Implant code (http://bifrost.lanl.gov/∼reed/).

I referee papers for several scientific journals, including; Journal of Applied Physics, Modelling and Simulation in Materials Science and Engineering, and Nuclear Instruments and Methods.

Interests and Activities:

I enjoy literature and cinema and I have an eclectic taste in music, attending concerts whenever possible. I enjoy traveling, and I traveled extensively in Europe after finishing my undergraduate degree course.

Since arriving at Los Alamos, I have taken advantage of the great natural resource provided by the New Mexican landscape; I am a keen snow-boarder, and hike and mountain-bike during the summer months.

References:

Available on Request.

Brief Research Biography

1991-92 MSc Dissertation:
Vibration Reduction for Helicopter Airframes by Structural Optimisation

This research was conducted during an industrial placement with the Defence Research Agency at RAE Farnborough. The project involved the use of finite element modeling and optimization to iteratively refine a model of the Lynx helicopter airframe, by modifying the mass and stiffness of components. The aim was to reduce vibration levels at specific locations within the airframe without compromising the strength of the structure.

Much of my time at Farnborough was spent debugging a prototype version of the analysis and optimization code. I designed optimization jobs, ran them on a Cray supercomputer and ultimately produced a modified airframe design that satisfied all strength criterion, with vibration levels reduced by 20%.

1992-95 PhD Thesis:
Dynamical Simulation of Multicomponent Carbon Based Materials

My thesis was concerned with research into the behavior of covalent materials using classical molecular dynamics (MD) simulation. During my research I wrote my own efficient and accurate MD code, optimized to run on UNIX workstations. This code runs at least four times faster than the MD program that was previously being used at Loughborough University, and is now being used there, at the University of Surrey, the University of Newcastle in Australia, and at Los Alamos.

A large part of my research concerned the interaction of molecules and ions with crystal surfaces. This required the development of models to describe the various types of interaction between the chemical species involved. Research was conducted in collaboration with experimental groups in order to gain understanding of, and explain, the atomic scale processes responsible for their observed results. I also developed computer visualization and animation techniques to gain understanding of dynamical processes within simulations. Computer generated movies illustrating typical simulation trajectories were produced to accompany papers and for use in presentations.

1996-99 Post Doctoral Fellow:
Atomic Scale Materials Modeling

My research was divided into two broad areas; *Radiation effects in materials*, and *Structure and dynamics of self-assembled systems*. Research into radiation effects in materials was directly related to materials problems of importance to industry and national laboratories. Topics included; modeling of dopant implants in silicon, behavior of polymer resists subject to ion implant, the interaction of energetic clusters with surfaces, radiation damage thresholds, and irradiation induced stress creation and relaxation in thin films. The principle result of this work has been the development and validation of a new, MD based, implant prediction code (named REED). The *alpha* version of this code was released to industry for full validation in January '98. Results of testing, and industry input were then used to guide the development of the *beta* version. Other research involved simulations to investigate the generation and release of stress in thin films subject to ion implant, or radiation damage. Results from these efforts were published, and presented at national conferences in the US, and led to an invitation to speak at an international conference.

Investigation of the structure and dynamics of self-assembled systems was related to proposed materials applications that took advantage of, or mimicked, the ability of nature to self-assemble complex structures. Research topics included; the growth and dynamical behavior of self-assembled monolayers (SAMs) on gold surfaces, and electrostatic interactions in biomaterials. My research involved the development of parallel and serial codes to conduct simulations at various levels of compromise between system size and model detail. This required the production of interaction models for classical simulations, based on data from electronic structure calculations. Results from these efforts were published, and presented at national conferences in the US. I was also a principal organizer of the Workshop on Self-Assembling and Biomimetic Materials, held at Los Alamos in December 1997. This three day meeting involved over 100 scientists from both within the Laboratory, and from U.S. and overseas academia, national labs and industry.

Publications:

1. **Energetic fullerene interactions with Si crystal surfaces**
   K. Beardmore, R. Smith, and R. P. Webb, *Modelling Simul. Mater. Sci. Eng.* **2** *(1994) 313-328.*

2. **The interaction of hydrogen with C_{60} fullerenes**
   K. Beardmore, R. Smith, A. Richter, and B. Mertesacker,
   J. Phys.: Condens. Matter **6** *(1994) 7351-7364.*

3. **Early stages of bump formation on the surface of ion-bombarded graphite**
   A. Gras-Marti, R. Smith, K. Beardmore, J. J. Jiménez-Rodríguez, V. Konoplev, and J. Ferrón,
   Comp. Mat. Science **3** *(1995) 413-422.*

4. **The interaction of C_{60} with hydrogen plasma**
   K. Beardmore, R. Smith, A. Richter, and B. Mertesacker, *Vacuum* **46** *(1995) 1091-1096.*

5. **Molecular dynamics simulations of particle surface interactions**
   R. Smith, K. Beardmore, and A. Gras-Marti, *Vacuum* **46** *(1995) 1195-1999.*

6. **Ion bombardment of polyethylene**
   K. Beardmore and R. Smith, *Nucl. Instrum. and Meth. B.* **102** *(1995) 223-227.*

7. **A molecular dynamics study of energetic particle impacts on carbon and silicon**
   R. Smith, K. Beardmore, A. Gras-Marti, R. Kirchner, and R. P. Webb,
   Nucl. Instrum. and Meth. B. **102** *(1995) 211-217.*

8. **An investigation of collision propagation in energetic ion initiated cascades in copper**
   I. R. Chakarov, R. P. Webb, R. Smith, and K. Beardmore,
   Nucl. Instrum. and Meth. B. **102** *(1995) 145-150.*

9. **C_{60} film growth and the interaction of fullerenes with bare and H terminated Si surfaces, studied by molecular dynamics**
   K. Beardmore and R. Smith, *Nucl. Instrum. and Meth. B.* **106** *(1995) 74-79.*

10. **Dynamical simulation of multicomponent carbon based materials**
    K. M. Beardmore, *Ph.D. Thesis, Loughborough University of Technology (1995).*

11. **Molecular dynamics studies of particle impacts with carbon-based materials**
    R. Smith and K. Beardmore, *Thin Solid Films* **272** *(1996) 255-270.*

12. **Empirical potentials for C-Si-H systems with application to C_{60} interactions with Si crystal surfaces**
    K. Beardmore and R. Smith, *Phil. Mag. A.* **74** *(1996) 1439-1466.*

13. **The growth of fullerite films: Experiment and computer simulation**
    K. Beardmore, R. Smith, A. Richter, and B. Winzer, *Mol. Mat.* **7** *(1996) 155-162.*

14. **The computer simulation of energetic particle-solid interactions**
    R. P. Webb, R. Smith, I. R. Chakarov, and K. Beardmore,
    Nucl. Instrum. and Meth. B. **112** *(1996) 99-104.*

15. **Phenomenological electronic stopping power model for molecular dynamics and Monte Carlo simulation of ion implantation into silicon**
    D. Cai, N. Grønbech-Jensen, C. M. Snell, and K. M. Beardmore, *Phys. Rev. B.* **54** *(1996) 17147-17157.*

16. **Molecular dynamics simulation of low energy boron and arsenic implant into silicon**
    K. M. Beardmore, D. Cai, and N. Grønbech-Jensen, in *Proceedings of Ion Implantation Technology, Austin, 1996*, edited by E. Ishida (IEEE **96TH8182**, 1997), pp. 535-538.

17. **An electronic stopping power model for monte carlo and molecular dynamics simulation of ion implantation into silicon**
    D. Cai, N. Grønbech-Jensen, C. M. Snell, K. M. Beardmore, S. Morris, and A. F. Tasch,
    in *Proceedings of Ion Implantation Technology, Austin, 1996*,
    edited by E. Ishida (IEEE **96TH8182**, 1997), pp. 543-546.

18. **Ab-initio calculations of the gold-sulfur interaction for alkanethiol monolayers**
K. M. Beardmore, J. D. Kress, A. R. Bishop, and N. Grønbech-Jensen,
Synthetic Metals **84** *(1997) 317-318.*

19. **Molecular dynamics simulation of self-assembled monolayers with defects**
K. M. Beardmore, N. Grønbech-Jensen, J. D. Kress, and A. N. Parikh,
Abstracts Of Papers Of The American Chemical Society **214** *(1997) 6.*

20. **Molecular dynamics simulation of 0.1–2 keV ion bombardment of Ni{100}**
R. Smith, B. King, and K. Beardmore, *Radiat. Eff. Defects Solids* **141** *(1997) 425-451.*

21. **Lekner summation of Coulomb interactions in partially periodic systems**
N. Grønbech-Jensen, G. Hummer, and K. M. Beardmore, *Molecular Physics* **92** *(1997) 941-945.*

22. **Low energy model for ion implantation of arsenic and boron into (100) single-crystal silicon**
B. J. Obradovic, S. J. Morris, M. Morris, S. Tian, G. Wang, K. Beardmore, C. Snell, J. Jackson, S. Baummann, and A. F. Tasch, in *Proceedings of Microelectronic Device Technology, Austin, 1997*, (SPIE-Int. Soc. Opt. Eng. **3212**, 1997), pp. 342-353.

23. **Low energy model for ion implantation of arsenic and boron into (100) single-crystal silicon**
B. J. Obradovic, S. J. Morris, M. Morris, S. Tian, G. Wang, K. Beardmore, C. Snell, C. Freer, and A. F. Tasch, in *Proceedings of 4th International Workshop on Measurement, Characterization and Modeling of Ultra-Shallow Doping Profiles in Semiconductors, Research Triangle Park, NC, 1997*, (Austin, TX, USA : Applied Mater. **49**, 1997), pp. 1-9.

24. **Determination of the headgroup-gold(111) potential surface for alkanethiol self-assembled monolayers by ab-initio calculation**
K. M. Beardmore, J. D. Kress, N. Grønbech-Jensen, and A. R. Bishop,
Chem. Phys. Lett. **286** *(1998) 40-45.*

25. **Efficient molecular dynamics scheme for the calculation of dopant profiles due to ion implantation**
K. M. Beardmore and N. Grønbech-Jensen, *Phys. Rev. E.* **57** *(1998) 7278-7287.*

26. **Simulation of phosphorus implantation into silicon with a single-parameter electronic stopping power model**
D. Cai, C. M. Snell, K. M. Beardmore, and N. Grønbech-Jensen, *Int. J. Mod. Phys. C.* **9** *(1998) 459-470.*

27. **Interactions between charged spheres in divalent counterion solution**
N. Grønbech-Jensen, K. M. Beardmore, and P. Pincus, *Physica A.* **261** *(1998) 74-81.*

28. **An efficient molecular dynamics scheme for predicting dopant implant profiles in semiconductors**
K. M. Beardmore and N. Grønbech-Jensen, *Nucl. Instrum. and Meth. B.* **153** *(1999) 391-397.*

29. **Characterization of chain molecular assemblies in long-chain, layered silver thiolates: A joint infrared spectroscopy and X-ray diffraction study**
A. N. Parikh, S. D. Gillmor, J. D. Beers, K. M. Beardmore, R. W. Cutts, and B. I. Swanson,
J. Phys. Chem. B. **103** *(1999) 2850-2861.*

30. **Stepwise assembly of silver(n-alkane)thiolates: an example of hierarchical or cooperative self-assembly**
J. D. Beers, A. N. Parikh, S. D. Gillmor, K. M. Beardmore, R. W. Cutts, and B. I. Swanson,
J. Young Investigators **1** *(1999) 1.*

31. **Predicting low energy dopant implant profiles in semiconductors using molecular dynamics**
K. M. Beardmore and N. Grønbech-Jensen, in *Proceedings of the Fifth International Symposium on Process Physics and Modeling in Semiconductor Technology*,
(Electrochemical Society, Pennington, 1999), pp. 3-17.

32. **Direct simulation of ion beam induced stressing and amorphization of silicon**
K. M. Beardmore and N. Grønbech-Jensen, in *Proceedings of the Fifth International Symposium on Process Physics and Modeling in Semiconductor Technology*,
(Electrochemical Society, Pennington, 1999), pp. 96-105.

33. **H-C_{60} and low energy H impact with fullerite**
R. Smith, K. Beardmore, and J. Belbruno, *J. Chem. Phys.* **111** *(1999) 9227-9232.*

34. **Direct simulation of ion beam induced stressing and amorphization of silicon**
K. M. Beardmore and N. Grønbech-Jensen, *Phys. Rev. B.* **60** *(1999) 12610-12616.*

Publications in preparation:

1. **The effect of surface potential on domain growth in alkanethiol monolayers**
N. Grønbech-Jensen, K. M. Beardmore, and A. N. Parikh, *(in preparation).*

2. **A complete model of implant energy loss using a consistent electron distribution**
N. Grønbech-Jensen, K. M. Beardmore, and B. Fraser, *(in preparation).*

3. **Determination of defect capture radii in silicon based on ab-inito calculations**
K. M. Beardmore, W. Windl, and F. Lin, *(in preparation).*

4. **Concentration profiles for seven dopant species implanted into Si(110) calculated using molecular dynamics simulation**
K. M. Beardmore and N. Grønbech-Jensen, *(in preparation).*

Selected Presentations:

Invited Talks:

1. **An efficient molecular dynamics scheme for predicting dopant implant profiles in semiconductors**
Computer Simulation Of Radiation Effects In Solids, Okayama, Japan, September 1998.

Talks:

1. **Ion bombardment of polyethylene**
Computer Simulation Of Radiation Effects In Solids, Santa Barbara, CA, USA, July 1994.

2. **Ab-initio calculations of the gold-sulfur interaction for alkanethiol monolayers**
International Conference On Synthetic Metals, Snowbird, UT, USA, July 1996.

3. **Dynamical simulation of perturbed systems of alkanethiols on gold surfaces**
American Vacuum Society Symposium, Philadelphia, PA, USA, October 1996.

4. **Molecular dynamics simulation of self-assembled monolayers with defects**
American Chemical Society Symposium, Las Vegas, NV, USA, September 1997.

5. **An efficient molecular dynamics scheme for predicting ultrashallow dopant implant profiles in semiconductors**
Materials Research Society Spring Meeting, San Francisco, CA, USA, April 1999.

6. **Direct simulation of ion beam induced stressing and amorphization of silicon**
Electrochemical Society Meeting, Seattle, WA, USA, May 1999.

Posters:

1. **Energetic fullerene interactions with Si crystal surfaces**
CCP5 Annual Meeting, Keele, Staffordshire, UK, September 1993.

2. **Fast algorithms for MD simulations**
Simulation Of Radiation Effects In Solids, Santa Barbara, CA, USA, July 1994.

3. **Molecular dynamics studies of C_{60} film growth and the interaction of fullerenes with bare and H terminated Si surfaces**
Ion Beam Modification of Materials, Canberra, ACT, Australia, February 1995.

4. **Molecular dynamics simulation of low energy boron and arsenic implant into silicon**
International Conference on Ion Implantation Technology, Austin, TX, USA, June 1996.

5. **Computer simulation of domain growth in self-assembled monolayers**
Workshop on Self-Assembling and Biomimetic Materials, Los Alamos, NM, USA, December 1997.

6. **An efficient molecular dynamics scheme for predicting dopant implant profiles in semiconductors**
   Materials Research Society Fall Meeting, Boston, MA, USA, November 1998.

7. **Direct simulation of ion beam induced stressing and amorphization of silicon**
   Materials Research Society Spring Meeting, San Francisco, CA, USA, April 1999.